Isophthalic acid, isobutyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C17H22O4/c1-12(2)8-9-20-16(18)14-6-5-7-15(10-14)17(19)21-11-13(3)4/h5-8,

InchiKey: LOOAYZQCMBQKDI-UHFFFAOYSA-N

Formula: C17H22O4

SMILES: CC(C)=CCOC(=O)c1cccc(C(=O)OCC(C)C)c1

Mol. weight [g/mol]: 290.35

Physical Properties

Property code	Value	Unit	Source
gf	-203.57	kJ/mol	Joback Method
hf	-556.60	kJ/mol	Joback Method
hfus	34.38	kJ/mol	Joback Method
hvap	74.34	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.622		Crippen Method
mcvol	237.210	ml/mol	McGowan Method
pc	1769.87	kPa	Joback Method
rinpol	2182.00		NIST Webbook
tb	776.20	K	Joback Method
tc	987.88	K	Joback Method
tf	430.57	K	Joback Method
vc	0.902	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.54	J/mol×K	776.20	Joback Method
cpg	694.83	J/mol×K	811.48	Joback Method
cpg	709.08	J/mol×K	846.76	Joback Method
cpg	722.30	J/mol×K	882.04	Joback Method
cpg	734.55	J/mol×K	917.32	Joback Method
cpg	745.83	J/mol×K	952.60	Joback Method
cpg	756.18	J/mol×K	987.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343934&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume